Proceedings of the Indian Academy of Sciences, Vol. VIII, No. 5, November 1938

ON AN INEQUALITY CONCERNING LATTICE SUMS.

BY

B. S. MADHAVA RAO and K. VENKATACHALA IYENGAR.

Reprinted from "The Proceedings of the Indian Academy of Sciences",
Vol. VIII, No. 5, Sec. A, 1938.

ON AN INEQUALITY CONCERNING LATTICE SUMS.

BY B. S. MADHAVA RAO
AND
K. VENKATACHALA IYENGAR.
(From the Department of Mathematics, University of Mysore, Bangalore.)

§ 1. *Introduction.*

THE present investigation arose out of an attempt to examine the suggestion put forward by Raman and Krishnan[1] that the optical anisotropy of the molecules of a liquid tends to diminish when the influence of the neighbouring molecular field is taken into consideration. We started with the model of a rhombic lattice of static dipoles, but it was soon found that this model was inadequate for the purpose on hand. There arose, however, in the course of the investigations some inequalities connected with lattice sums which presented many points of mathematical interest. Specially in view of the fact that, although the actual evaluation of lattice sums figures prominently in the literature, the question of inequalities of such sums has nowhere been treated, we have thought it desirable to have them placed on record here.

§ 2. *Statement of the inequality.*

Consider a rhombic lattice with the constants a, b, c, and let the origin be chosen at any one molecule situated at a corner of the lattice. The co-ordinates of any other molecule can be taken as $(n_1 a, n_2 b, n_3 c)$ where n_1, n_2, n_3 are integers. The potential due to a doublet at r is given by

$$\left(p, \text{grad } \frac{1}{r}\right) = \frac{xp_x + yp_y + zp_z}{r^3},$$

where p is the moment of the dipole. Hence the components of the force due to this potential are given by

$$\mathrm{F}_x = -\frac{\partial\phi}{\partial x} = \frac{1}{r^5}\left\{p_x\,(3x^2 - r^2) + 3xyp_y + 3zxp_z\right\}$$

and the total force

$$\mathrm{E}_x = \Sigma\,\mathrm{F}_x = \Sigma\,\frac{1}{r^5}\left\{p_x\,(2n_1^2a^2 - n_2^2b^2 - n_3^2c^2) + 3n_1n_2\,ab\,p_y + 3n_1n_3\,ca\,p_z\right\}$$

$$= \Sigma\,\frac{\{p_x\,(2n_1^2a^2 - n_2^2b^2 - n_3^2c^2) + 3n_1n_2\,ab\,p_y + 3n_3n_1\,ca\,p_z\}}{(a^2n_1^2 + b^2n_2^2 + c^2n_3^2)^{\frac{5}{2}}}$$

$$= \mathrm{S}_{11}\,p_x + \mathrm{S}_{12}\,p_y + \mathrm{S}_{13}\,p_z.$$

From considerations of symmetry $S_{12} = S_{13} = 0$. It might also be noticed that for a cubic lattice ($a = b = c$) we also have $S_{11} = 0$. In an exactly similar manner we can introduce the sums S_{22} and S_{33}. The difference

$$S_{11} - S_{22} = 3 \sum_{n_1, n_2, n_3} \frac{(a^2 n_1^2 - b^2 n_2^2)}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{\frac{5}{2}}}.$$

The problem with which we are concerned in this paper is to find out whether this difference is positive or negative when $a > b$. For this purpose we consider the more general series

$$f(a, b, c) = \Sigma \frac{a^\lambda n_1^2}{(a^2 n_1^2 + b_2 n_2^2 + c^2 n_3^2)^r}, \tag{1}$$

examine its convergence, and then the inequalities $f(a, b, c) \gtrless f(b, a, c)$ in the case of three and two dimensions (*i.e.*, a plane lattice). The results are given in the following two sections.

§ 3. *Proof in the case of a rhombic lattice.*

The summation in (1) can be assumed to be taken over all positive and negative values of n_1, n_2, n_3 excluding $n_1 = n_2 = n_3 = 0$. The terms of the series are less than the corresponding terms of the series

$$\Sigma \frac{a^{\lambda - 2}}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{r-1}}.$$

Comparing this with

$$\Sigma \frac{1}{(n_1^2 + n_2^2 + n_3^2)^{r-1}}$$

we see that the original series converges for $r > 5/2$. Let $a/b = \mu > 1$. Then we prove the following results.

$$f(a, b, c) > f(b, a, c) \qquad \text{if } \lambda \geqslant 2r \tag{2}$$

$$f(a, b, c) < f(b, a, c) \qquad \text{if } \lambda \leqslant 2r - 3. \tag{3}$$

The method of proof adopted is the well-known process of transformation of series due to Kronecker. Now

$$\frac{\Gamma r}{\alpha^r} = \int_0^\infty e^{-\alpha t}\, t^{r-1}\, dt\,; \quad \alpha > 0.$$

Take $\alpha = \pi (a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)$. Then we obtain

$$\int_0^\infty e^{-\pi (a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)\, t} \,.\, t^{r-1}\, dt = \frac{\Gamma r}{\pi^r} \cdot \frac{1}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^r}.$$

Hence,

$$f(a, b, c) = \frac{a^{\lambda}\,\pi^{r}}{\Gamma r} \int_0^\infty \Sigma\, n_1^2\, e^{-\pi(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)t} \,.\, t^{r-1}\, dt, \tag{4}$$

the validity of the operation effected above being too well known to be repeated here. Now let,

$$\omega(x) = \sum_{-\infty}^{\infty} e^{-n^2 \pi x}, \text{ then}$$

$$\omega'(x) = -\pi \,\Sigma\, n^2 e^{-n^2 \pi x}.$$

We can write (4) in the form,

$$f(a, b, c) = \frac{a^{\lambda}\,\pi^{r-1}}{\Gamma r} \int_0^\infty \Sigma\, \pi n_1^2\, e^{-\pi a^2 n_1^2 t} .\; \Sigma\, e^{-\pi b^2 n_2^2 t} .\; \Sigma\, e^{-\pi c^2 n_3^2 t} \,.\, t^{r-1}\, dt.$$

$$= -\frac{a^{\lambda}\,\pi^{r-1}}{\Gamma r} \int_0^\infty \omega(b^2 t)\, \omega^1(a^2 t)\, \omega(c^2 t)\, t^{r-1}\, dt.$$

Taking $a^2 t = v$, we get

$$f(a, b, c) = -\frac{\pi^{r-1}\, a^{\lambda-2r}}{\Gamma r} \int_0^\infty \omega\left(\frac{b^2 v}{a^2}\right) \omega\left(\frac{c^2 v}{a^2}\right) \omega'(v)\, v^{r-1}\, dv \tag{5}$$

In an exactly similar manner we obtain,

$$f(b, a, c) = -\frac{\pi^{r-1}\, b^{\lambda-2r}}{\Gamma r} \int_0^\infty \omega\left(\frac{a^2 v}{b^2}\right) \omega\left(\frac{c^2 v}{b^2}\right) \omega'(v)\, v^{r-1}\, dv \tag{6}$$

$f(a, b, c) - f(b, a, c) = \mathrm{A}.$

$$\int_0^\infty \omega'(v)\, v^{r-1} \left\{ \omega(\mu^2 v)\, \omega\left(\frac{c^2 v}{b^2}\right) - \mu^{\lambda-2r}\, \omega\left(\frac{v}{\mu^2}\right) \omega\left(\frac{c^2 v}{a^2}\right) \right\} dv \tag{7}$$

where $\mu = \dfrac{a}{b} > 1$, and A is a positive constant.

Now we show that the integrand in (7) is positive for $\lambda \geqslant 2r$, and negative for $\lambda \leqslant 2r - 3$, for all values of v. Since $\mu > 1$

$$\mu^2 v > \frac{v}{\mu^2} \text{ and } \frac{c^2 v}{b^2} > \frac{c^2 v}{a^2}.$$

From the fact that $\omega(x)$ is a decreasing function it follows that

$$\omega(\mu^2 v)\, \omega\left(\frac{c^2 v}{b^2}\right) < \omega\left(\frac{v}{\mu^2}\right) \omega\left(\frac{c^2 v}{a^2}\right).$$

Hence, if $\lambda \geqslant 2r$,

$$\omega(\mu^2 v)\, \omega\left(\frac{c^2 v}{b^2}\right) < \mu^{\lambda-2r}\, \omega\left(\frac{v}{\mu^2}\right) \omega\left(\frac{c^2 v}{a^2}\right).$$

Further, we observe that $\omega'(v)$ is throughout negative and hence the integrand is throughout positive. This proves (2).

To prove (3), we apply the functional equation of $\omega(x)$, *viz.*,

$$\omega(x) = \frac{1}{\sqrt{x}}\,\omega\left(\frac{1}{x}\right)$$

from which we have,

$$\omega(\mu^2 v) = \frac{1}{\mu\sqrt{v}}\,\omega\left(\frac{1}{\mu^2 v}\right);\ \omega\left(\frac{c^2 v}{b^2}\right) = \frac{b}{c\sqrt{v}}\,\omega\left(\frac{b^2}{c^2 v}\right).$$

$$\omega\left(\frac{v}{\mu^2}\right) = \frac{\mu}{\sqrt{v}}\,\omega\left(\frac{\mu^2}{v}\right);\ \omega\left(\frac{c^2 v}{a^2}\right) = \frac{a}{c\sqrt{v}}\,\omega\left(\frac{a^2}{c^2 v}\right).$$

Hence the expression inside the brackets in the integrand of (7) is equal to

$$\frac{b}{c\mu v}\,\omega\left(\frac{1}{\mu^2 v}\right)\omega\left(\frac{b^2}{c^2 v}\right) - \frac{a\mu^{\lambda-2r+1}}{cv}\,\omega\left(\frac{\mu^2}{v}\right)\omega\left(\frac{a^2}{e^2 v}\right)$$

$$= \frac{b}{c\mu v}\left\{\omega\left(\frac{1}{\mu^2 v}\right)\omega\left(\frac{b^2}{c^2 v}\right) - \mu^{\lambda-2r+3}\,\omega\left(\frac{\mu^2}{v}\right)\omega\left(\frac{a^2}{c^2 v}\right)\right\} \tag{8}$$

Now

$$\frac{1}{\mu^2 v} < \frac{\mu^2}{v};\ \frac{b^2}{c^2 v} < \frac{a^2}{\iota^2 v};\quad \text{therefore}$$

$$\omega\left(\frac{1}{\mu^2 v}\right) > \omega\left(\frac{\mu^2}{v}\right),\ \text{and}\ \omega\left(\frac{b^2}{c^2 v}\right) < \omega\left(\frac{a^2}{c^2 v}\right).$$

Hence, if $\lambda \leqslant 2r - 3$, it follows that the expression inside the brackets in (8) is positive. Hence in this case the integrand in (7) is throughout negative, and this proves (3). In particular we obtain, for $\epsilon > 0$, the inequalities

$$\Sigma \frac{a^{5+2\epsilon}\,n_1^2}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{\frac{5}{2}+\epsilon}} > \Sigma \frac{b^{5+2\epsilon}\,n_2^2}{(a^2 n_1^2 + b^2 n_1^2 + c^2 n_3^2)^{\frac{5}{2}+\epsilon}}, \tag{9}$$

and,

$$\Sigma \frac{a^2 n_1^2}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{\frac{5}{2}+\epsilon}} < \Sigma \frac{b^2 n_2^2}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{\frac{5}{2}+\epsilon}} \tag{10}$$

which answers the question raised in § 2.

§ 4. *The case of the plane lattice.*

In this case we put $c = 0$, and take $r > 3/2$ for the convergence of the series that arises. The discussion for (2) is the same as before. The corresponding expression obtained in this case is

$$f(a, b) - f(b, a) = A\int_0^\infty \omega'(x)\,x^{r-1}\left\{\omega(\mu^2 x) - \mu^{\lambda-2r}\,\omega\left(\frac{x}{\mu^2}\right)\right\} dx \cdots \tag{11}$$

where A is some positive constant. Now, we have

$$\omega\,(\mu^2 x) = \frac{1}{\mu\sqrt{x}}\,\omega\left(\frac{1}{\mu^2 x}\right), \text{ and } \omega\left(\frac{x}{\mu^2}\right) = \frac{\mu}{\sqrt{x}}\,\omega\left(\frac{\mu^2}{x}\right),$$

and the expression within the brackets in (11) can be written as

$$\frac{1}{\mu\sqrt{x}}\left\{\omega\left(\frac{1}{\mu^2 x}\right) - \mu^{\lambda - 2r + 2}\,\omega\left(\frac{\mu^2}{x}\right)\right\}.$$

Since

$$\frac{1}{\mu^2 x} < \frac{\mu^2}{x},\quad \omega\left(\frac{1}{\mu^2 x}\right) > \omega\left(\frac{\mu^2}{x}\right).$$

Hence, if $\lambda \leqslant 2r - 2$ we obtain that this is throughout positive, *i.e.*, the integrand is throughout negative. Thus the inequality (3), $f\,(a, b) < f\,(b, a)$ is valid even when $\lambda \leqslant 2r - 2$, unlike the case of three dimensions. In particular we may notice the following inequalities

$$\Sigma\,\frac{a^{3-\epsilon}\,n_1^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{5}{2}}} < \Sigma\,\frac{b^{3-\epsilon}\,n_2^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{5}{2}}} \quad (\epsilon > 0) \tag{12}$$

where, if $\epsilon = 1$, we get (2)

$$\Sigma\,\frac{a^2 n_1^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{5}{2}}} < \Sigma\,\frac{b^2 n_2^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{5}{2}}} \tag{12$'$}$$

i.e., $S_{11} < S_{22}$ if $a > b$. Also

$$\Sigma\,\frac{a^{1+2\rho-\epsilon}.n_1^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{3}{2}+\rho}} < \Sigma\,\frac{b^{1+2\rho-\epsilon}.n_2^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{3}{2}+\rho}} \tag{13}$$

$$\Sigma\,\frac{a^{3+2\rho+\epsilon}.n_1^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{3}{2}+\rho}} > \Sigma\,\frac{b^{3+2\rho+\epsilon}.n_2^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2})^{\frac{3}{2}+\rho}} \tag{14}$$

We might observe, in conclusion, that the method adopted in the previous section can be applied to the very general series

$$f\,(a, b, c, \cdots, k) = \Sigma\,\frac{a^\lambda n_1^{\,2}}{(a^2 n_1^{\,2} + b^2 n_2^{\,2} + \cdots + k^2 n_k^{\,2})^r},$$

and leads to the results that while (2) is valid, the inequality (3) is valid for $\lambda \leqslant 2r - k$. However, when $2r \geqslant \lambda \geqslant 2r - k$, the method we have adopted does not yield any definite result.

REFERENCES.

1. Raman, C. V., and Krishnan, K. S. *Proc. Roy. Soc.*, (A), 1927, **117**, 1 and 589.

2. A direct proof of (12′) was communicated to us by Dr. S. S. Pillai of Annamalai University.

The
BANGALORE
PRESS
LAKE VIEW
MYSORE RD
BANGALORE
CITY